

# Broad comp search.

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LOGINID:ssptayvv1621

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS	4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS	5	AUG 30	CA(SM)/CAPLUS(SM) Austrian patent law changes
NEWS	6	SEP 11	CA/CAPLUS enhanced with more pre-1907 records
NEWS	7	SEP 21	CA/CAPLUS fields enhanced with simultaneous left and right truncation
NEWS	8	SEP 25	CA(SM)/CAPLUS(SM) display of CA Lexicon enhanced
NEWS	9	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS	10	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS	11	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS	12	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS	13	OCT 19	E-mail format enhanced
NEWS	14	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS	15	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS	16	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS	17	OCT 30	CHEMLIST enhanced with new search and display field
NEWS	18	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS	19	NOV 10	CA/CAPLUS F-Term thesaurus enhanced
NEWS	20	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS	21	NOV 13	CA/CAPLUS pre-1967 chemical substance index entries enhanced with preparation role
NEWS	22	NOV 20	CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS	23	NOV 20	CA/CAPLUS to MARPAT accession number crossover limit increased to 50,000
NEWS	24	NOV 20	CA/CAPLUS patent kind codes will be updated
NEWS	25	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS	26	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS EXPRESS			NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items
NEWS IPC8			For general information regarding STN implementation of IPC 8
NEWS X25			X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 09:02:54 ON 14 DEC 2006

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 09:03:07 ON 14 DEC 2006

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STRUCTURE FILE UPDATES: 13 DEC 2006 HIGHEST RN 915360-23-5

DICTIONARY FILE UPDATES: 13 DEC 2006 HIGHEST RN 915360-23-5

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10540749-broader.str

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 09:03:26 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 13857 TO ITERATE

14.4% PROCESSED 2000 ITERATIONS

31 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 270088 TO 284192

PROJECTED ANSWERS: 3416 TO 5174

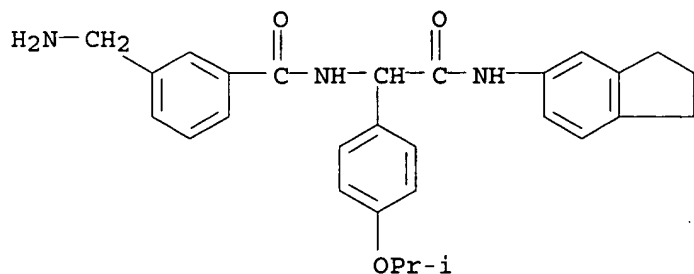
L2 31 SEA SSS SAM L1

=> d l2 scan

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzeneacetamide,  $\alpha$ -[[3-(aminomethyl)benzoyl]amino]-N-(2,3-dihydro-1H-inden-5-yl)-4-(1-methylethoxy)-(9CI)

MF C28 H31 N3 O3  
CI COM

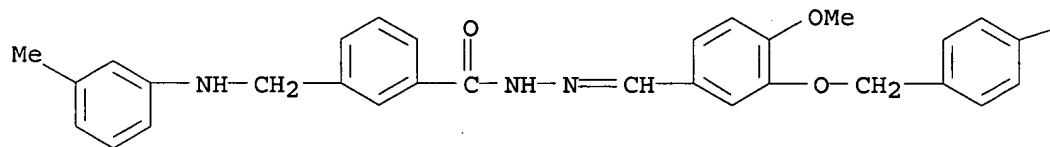


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN  
IN Benzoic acid, 3-[[[(3-methylphenyl)amino]methyl]-, [[4-methoxy-3-[(4-nitrophenyl)methoxy]phenyl]methylene]hydrazide (9CI)  
MF C30 H28 N4 O5

PAGE 1-A



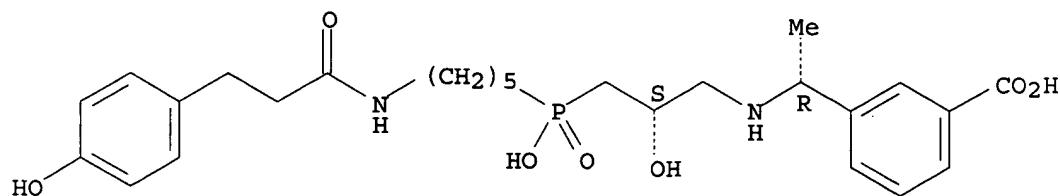
PAGE 1-B

—NO<sub>2</sub>

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN  
IN Benzoic acid, 3-[1-[[2-hydroxy-3-[hydroxy[5-[[3-(4-hydroxyphenyl)-1-oxopropyl]amino]pentyl]phosphinyl]propyl]amino]ethyl]-, [S-(R\*,S\*)]- (9CI)  
MF C26 H37 N2 O7 P

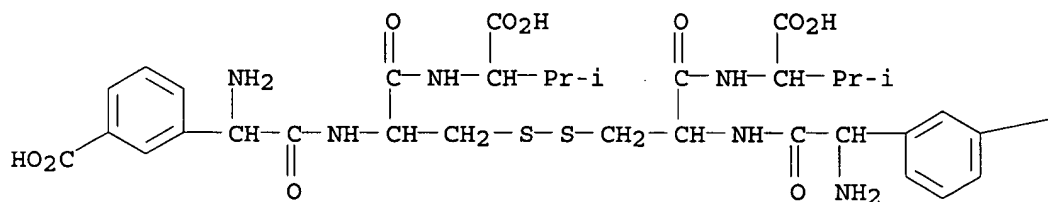
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN  
 IN D-Valine, 2-(3-carboxyphenyl)glycyl-L-cysteinyl-, bimol.  
 (2→2')-disulfide (9CI)  
 MF C34 H44 N6 O12 S2

PAGE 1-A

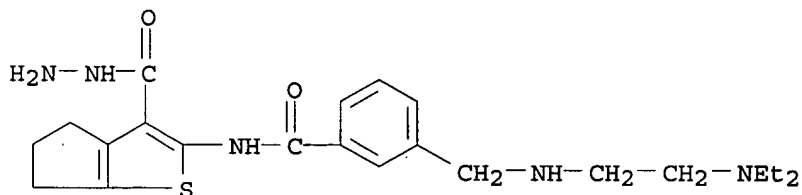


PAGE 1-B

—CO<sub>2</sub>H

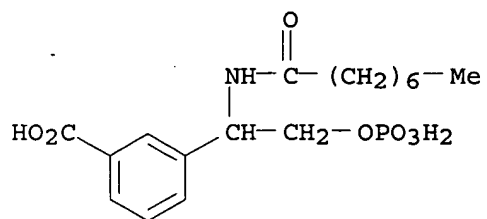
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN  
 IN 4H-Cyclopenta[b]thiophene-3-carboxylic acid, 2-[[3-[[2-(diethylamino)ethyl]amino]methyl]benzoyl]amino]-5,6-dihydro-, hydrazide (9CI)  
 MF C22 H31 N5 O2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN  
 IN Benzoic acid, 3-[1-[(1-oxooctyl)amino]-2-(phosphonooxy)ethyl]-, trisodium salt (9CI)  
 MF C17 H26 N O7 P . 3 Na



3 Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l1 full

FULL SEARCH INITIATED 09:04:34 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 279585 TO ITERATE

100.0% PROCESSED 279585 ITERATIONS

3239 ANSWERS

SEARCH TIME: 00.00.02

L3 3239 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

167.82

168.03

FILE 'CAPLUS' ENTERED AT 09:04:44 ON 14 DEC 2006

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FILE COVERS 1907 - 14 Dec 2006 VOL 145 ISS 25

FILE LAST UPDATED: 13 Dec 2006 (20061213/ED)

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<http://www.cas.org/infopolicy.html>

=> s l3 and friedel

757 L3

17141 FRIEDEL

L4

1 L3 AND FRIEDEL

=> d l4 ibib abs hitstr

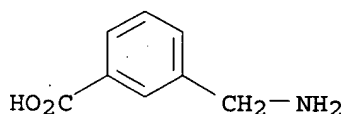
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:324185 CAPLUS

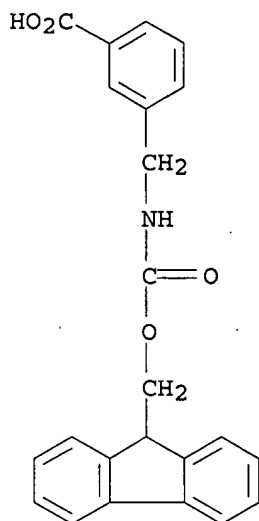
DOCUMENT NUMBER: 120:324185  
 TITLE: Design and Synthesis of a Biologically Active Antibody Mimic Based on an Antibody-Antigen Crystal Structure  
 AUTHOR(S): Smythe, M. L.; von Itzstein, M.  
 CORPORATE SOURCE: Victorian College of Pharmacy, Monash University, Parkville, 3052, Australia  
 SOURCE: Journal of the American Chemical Society (1994), 116(7), 2725-33  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The crystal structure of an N9 sialidase (antigen)-NC41 (antibody) complex was used to design a low mol. weight cyclopeptide that mimics the binding function of the macromol. antibody. The components of recognition between the antibody and the protein antigen have been analyzed from the energy-refined crystal complex. From this anal., four amino acid residues on the antibody binding surface, which make direct contact with the active-site loop 368-370 of the antigen, were identified as contributing the majority of the binding energy of the protein. The designed target cyclo(Phe-Amb-Glu-Asp-Asn) [Amb = 3-(aminomethyl)benzoic acid], a constrained cyclic peptide that mimics the receptor-bound conformation of these amino acids, was prepared and found to inhibit N9 sialidase activity with a  $K_i$  of  $1 + 10^{-4}$  M.

IT 2393-20-6P, 3-(Aminomethyl)benzoic acid  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and fluorenylmethoxycarbonylation of)  
 RN 2393-20-6 CAPLUS  
 CN Benzoic acid, 3-(aminomethyl)- (9CI) (CA INDEX NAME)



IT 155369-11-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and solid-phase peptide coupling reactions of, in preparation of  
 cyclopeptide antibody mimic)  
 RN 155369-11-2 CAPLUS  
 CN Benzoic acid, 3-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]methyl]- (9CI)  
 (CA INDEX NAME)



=> s l3 and acylation

757 L3

59127 ACYLATION

L5

19 L3 AND ACYLATION

=> d l5 ibib abs hitstr

L5 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:333345 CAPLUS

DOCUMENT NUMBER: 144:350709

TITLE: Pyrazolopyrimidines as protein kinase B inhibitors, their preparation, pharmaceutical compositions, and use in therapy

INVENTOR(S): Maier, Thomas; Zuelch, Armin; Ciossek, Thomas; Baer, Thomas; Beckers, Thomas

PATENT ASSIGNEE(S): Altana Pharma AG, Germany

SOURCE: PCT Int. Appl., 114 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006027346	A2	20060316	WO 2005-EP54366	20050905
WO 2006027346	A3	20060803		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.:

EP 2004-104283

A 20040906

OTHER SOURCE(S):

MARPAT 144:350709

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention relates to pyrazolopyrimidine derivs. I, which are inhibitors of protein kinase B (PKB)/Akt. In compds. I, R1 is (un)substituted aryl or (un)substituted heteroaryl; R2 is H, halo, or C1-4 alkyl; R3 is selected from (un)substituted amino-C1-4 alkyl, heterocycl-yl-C1-4 alkyl, (un)substituted Ph, (un)substituted phenyl-C1-4 alkyl, (un)substituted heteroaryl, etc.; and R4 is H or halo; including salts thereof. The invention also relates to the preparation of I, pharmaceutical compns. comprising one or more compds. of formula I together with a pharmaceutically acceptable carrier or diluent, as well as to the use of the compns. for the treatment, prevention, or amelioration of benign or malignant neoplasia, such as cancer. Deprotonation of 4-methoxybut-3-en-2-one followed by acylation with 4-bromobenzoyl chloride gave pentenedione II, which underwent heterocyclization with thiosemicarbazide, S-methylation, and oxidation resulting in the formation of sulfonylpyrazolopyrimidine III. Compound III was substituted with tert-Bu N-(4-aminophenyl)carbamate followed by deprotection, amidation with N-Boc-4-(2-aminoethyl)benzoic acid, and deprotection to give the hydrochloride salt of pyrazolopyrimidine IV. Five compds. of the invention, e.g., IV, inhibit Akt1 with IC50 values below 4.03  $\mu$ M and exhibit antiproliferative/cytotoxic activity with IC50 values below 16.9  $\mu$ M and 13.6  $\mu$ M in assays using MCF7 and MDA468 cancer cell lines, resp.

IT 881215-02-7P, 3-Aminomethyl-N-[3-((5-(Dibenzofuran-4-yl)pyrazolo[1,5-c]pyrimidin-7-yl)amino)phenyl]benzamide trifluoroacetate  
881215-06-1P, 3-Aminomethyl-N-[4-((5-(Dibenzofuran-4-yl)pyrazolo[1,5-c]pyrimidin-7-yl)amino)phenyl]benzamide trifluoroacetate  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(drug candidate; preparation of pyrazolopyrimidines as protein kinase B inhibitors)

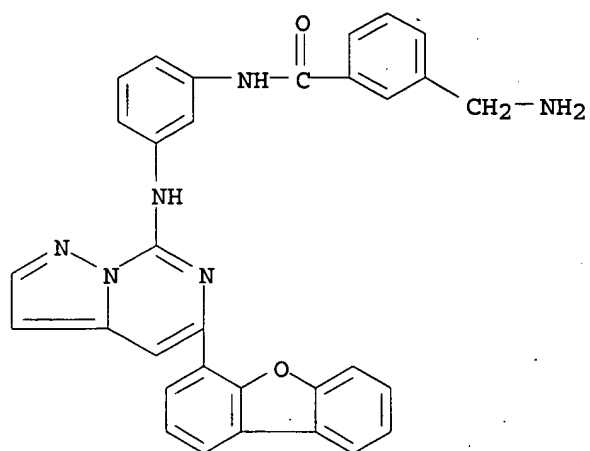
RN 881215-02-7 CAPLUS

CN Benzamide, 3-(aminomethyl)-N-[3-[[5-(4-dibenzofuranyl)pyrazolo[1,5-c]pyrimidin-7-yl]amino]phenyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 881215-01-6

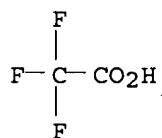
CMF C32 H24 N6 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



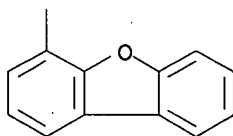
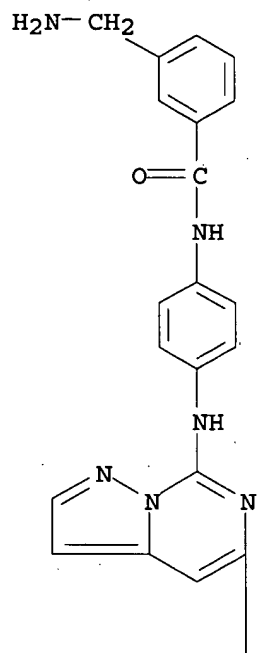
RN 881215-06-1 CAPLUS

CN Benzamide, 3-(aminomethyl)-N-[4-[[5-(4-dibenzofuranyl)pyrazolo[1,5-c]pyrimidin-7-yl]amino]phenyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 881215-05-0

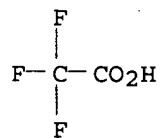
CMF C32 H24 N6 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



=> s l3 and aromatic substitution

757 L3

231823 AROMATIC

259602 SUBSTITUTION

2102 AROMATIC SUBSTITUTION

(AROMATIC(W) SUBSTITUTION)

L6

0 L3 AND AROMATIC SUBSTITUTION

=> s l3 and substitution

757 L3

## 259602 SUBSTITUTION

L7 28 L3 AND SUBSTITUTION

=&gt; s l7 or l5

L8 45 L7 OR L5

=&gt; s l8 not py &gt; 2003

3632143 PY &gt; 2003

L9 31 L8 NOT PY &gt; 2003

=&gt; d l9 ibib abs hitstr

L9 ANSWER 1 OF 31 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:478576 CAPLUS

DOCUMENT NUMBER: 139:175717

TITLE: Recognition and resistance in TEM  $\beta$ -lactamase

AUTHOR(S): Wang, Xiaojun; Minasov, George; Blazquez, Jesus;

Caselli, Emilia; Prati, Fabio; Shoichet, Brian K.

CORPORATE SOURCE: Department of Pharmaceutical Chemistry, University of California San Francisco, San Francisco, CA, 94143, USA

SOURCE: Biochemistry (2003), 42(28), 8434-8444

CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Developing antimicrobials that are less likely to engender resistance has become an important design criterion as more and more drugs fall victim to resistance mutations. One hypothesis is that the more closely an inhibitor resembles a substrate, the more difficult it will be to develop resistant mutations that can at once disfavor the inhibitor and still recognize the substrate. To investigate this hypothesis, 10 transition-state analogs, of greater or lesser similarity to substrates, were tested for inhibition of TEM-1  $\beta$ -lactamase, the most widespread resistance enzyme to penicillin antibiotics. The inhibitors were also tested against four characteristic mutant enzymes: TEM-30, TEM-32, TEM-52, and TEM-64. The inhibitor most similar to the substrate, compound 10, was the most potent inhibitor of the WT enzyme, with a  $K_i$  value of 64 nM. Conversely, compound 10 was the most susceptible to the TEM-30 (R244S) mutant, for which inhibition dropped by over 100-fold. The other inhibitors were relatively impervious to the TEM-30 mutant enzyme. To understand recognition and resistance to these transition-state analogs, the structures of four of these inhibitors in complex with TEM-1 were determined by x-ray crystallog. These structures suggest a structural basis for distinguishing inhibitors that mimic the acylation transition state and those that mimic the deacylation transition state; they also suggest how TEM-30 reduces the affinity of compound 10. In cell culture, this inhibitor reversed the resistance of bacteria to ampicillin, reducing min. inhibitory concns. of this penicillin by between 4- and 64-fold, depending on the strain of bacteria. Notwithstanding this activity, the resistance of TEM-30, which is already extant in the clinic, suggests that there can be resistance liabilities with substrate-based design.

IT 497258-67-0D, complexes with TEM-1  $\beta$ -lactamase

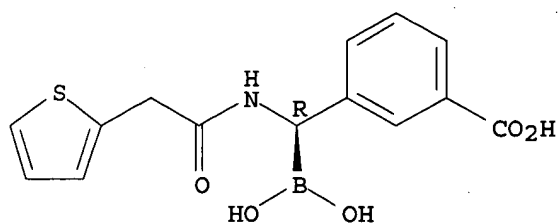
RL: PRP (Properties)

(crystal structure of TEM-1  $\beta$ -lactamase-transition state analog complexes)

RN 497258-67-0 CAPLUS

CN Benzoic acid, 3-[(R)-borono[(2-thienylacetyl)amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



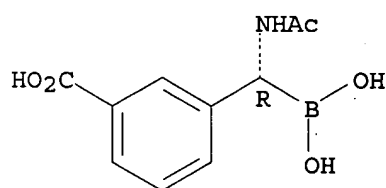
IT 497258-66-9 497258-67-0 497258-68-1

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(transition state analog recognition and inhibition by TEM  
β-lactamase mutants in relation to antibiotic resistance)

RN 497258-66-9 CAPLUS

CN Benzoic acid, 3-[(R)-(acetylamino)boronomethyl]- (9CI) (CA INDEX NAME)

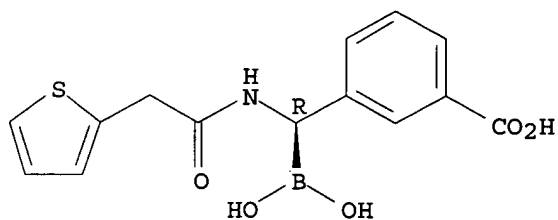
Absolute stereochemistry.



RN 497258-67-0 CAPLUS

CN Benzoic acid, 3-[(R)-borono[(2-thienylacetyl)amino]methyl]- (9CI) (CA INDEX NAME)

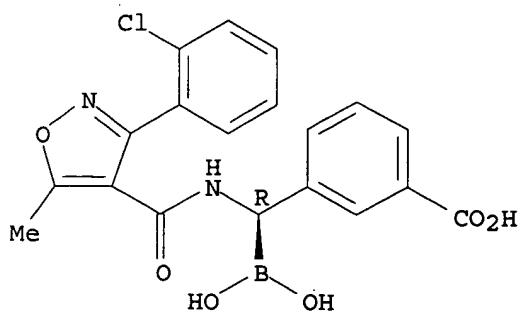
Absolute stereochemistry. Rotation (-).



RN 497258-68-1 CAPLUS

CN Benzoic acid, 3-[(R)-borono[[[3-(2-chlorophenyl)-5-methyl-4-isoxazolyl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT:

44

THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
33.01	201.04

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-2.25	-2.25

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 09:12:41 ON 14 DEC 2006

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DICTIONARY FILE UPDATES: 13 DEC 2006 HIGHEST RN 915360-23-5

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

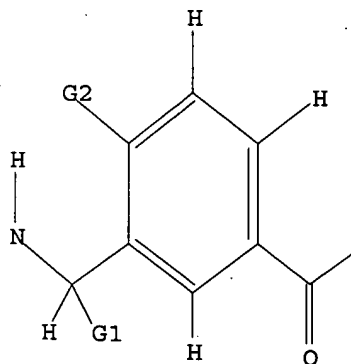
Uploading C:\Program Files\Stnexp\Queries\10540749-broader2.str

L10 STRUCTURE UPLOADED

=> d l10

L10 HAS NO ANSWERS

L10 STR



G1 H, Me, Et, n-Pr, i-Pr, n-Bu, i-Bu

G2 H, X

Structure attributes must be viewed using STN Express query preparation.

=> s l10

SAMPLE SEARCH INITIATED 09:13:24 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 2433 TO ITERATE

82.2% PROCESSED 2000 ITERATIONS 6 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 45702 TO 51618  
PROJECTED ANSWERS: 6 TO 307

L11 6 SEA SSS SAM L10

=> s l10 full

FULL SEARCH INITIATED 09:13:29 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 49225 TO ITERATE

100.0% PROCESSED 49225 ITERATIONS 117 ANSWERS  
SEARCH TIME: 00.00.01

L12 117 SEA SSS FUL L10

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
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	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.25

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=> s l12

L13 49 L12

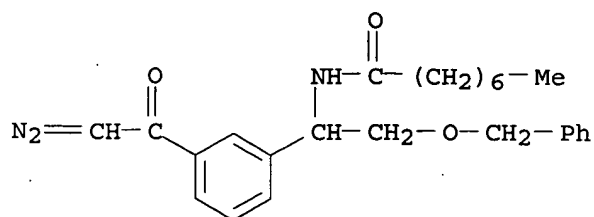
=> acylation and l13  
 ACYLATION IS NOT A RECOGNIZED COMMAND  
 The previous command name entered was not recognized by the system.  
 For a list of commands available to you in the current file, enter  
 "HELP COMMANDS" at an arrow prompt (=>).

=> s l13 and acylation  
 59127 ACYLATION  
 L14 0 L13 AND ACYLATION

=> s l13 not py > 2002  
 4688838 PY > 2002  
 L15 14 L13 NOT PY > 2002

=> d l15 ibib abs hitstr 1-  
 YOU HAVE REQUESTED DATA FROM 14 ANSWERS - CONTINUE? Y/(N):y

L15 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2002:823424 CAPLUS  
 DOCUMENT NUMBER: 139:6655  
 TITLE: Highly potent inhibitors of TNF- $\alpha$  production.  
 Part I. Discovery of new chemical leads and Their  
 structure-Activity relationships  
 AUTHOR(S): Matsui, Toshiaki; Kondo, Takashi; Nishita, Yoshitaka;  
 Itadani, Satoshi; Nakatani, Shingo; Omawari,  
 Nagashige; Sakai, Masaru; Nakazawa, Shuichi; Ogata,  
 Akihito; Mori, Hideaki; Terai, Kouichiro; Kamoshima,  
 Wataru; Ohno, Hiroyuki; Obata, Takaaki; Nakai, Hisao;  
 Toda, Masaaki  
 CORPORATE SOURCE: Fukui Research Institute, Ono Pharmaceutical Co.,  
 Ltd., Sakai, Fukui, 913-8638, Japan  
 SOURCE: Bioorganic & Medicinal Chemistry (2002), 10(12),  
 3757-3786  
 CODEN: BMECEP; ISSN: 0968-0896  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:6655  
 AB Discovery of new chemical leads of inhibitors for TNF- $\alpha$  production starting  
 from the chemical modification of 2-(octanoylamino)-2-phenylethyl disodium  
 phosphate (I) is reported. Further biol. studies of I to disclose the  
 site of its action strongly suggested that I inhibits LPS-induced  
 TNF- $\alpha$  expression in the liver and spleen of mice.  
 Structure-activity relationships (SARs) are also discussed and full  
 details including the chemical are reported.  
 IT 532986-93-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of alkylamino aryl disodium phosphates and their  
 structure-activity relationships as highly potent inhibitors of  
 TNF- $\alpha$  production)  
 RN 532986-93-9 CAPLUS  
 CN Octanamide, N-[1-[3-(diazoacetyl)phenyl]-2-(phenylmethoxy)ethyl]- (9CI)  
 (CA INDEX NAME)

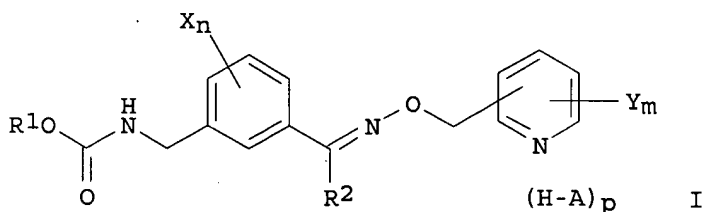


REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2002:615570 CAPLUS  
DOCUMENT NUMBER: 137:140441  
TITLE: Preparation of iminooxymethylpyridine compounds and agricultural or horticultural fungicides  
INVENTOR(S): Fukumoto, Shunichiro; Shibayama, Atsushi; Shibata, Masaru; Yonekura, Norihisa; Takagaki, Makiichi; Miura, Ichiro; Nagayama, Kouzou  
PATENT ASSIGNEE(S): Kumiai Chemical Industry Co., Ltd., Japan; Ihara Chemical Industry Co., Ltd.  
SOURCE: PCT Int. Appl., 33 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002062759	A1	20020815	WO 2002-JP792	20020131
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			JP 2001-26827	A 20010202

OTHER SOURCE(S): MARPAT 137:140441  
GI



AB Novel benzylideneiminooxymethylpyridine compound derivs. having the following general formula (I; wherein X represents halogeno, C1-6 alkyl, C1-6 alkoxy, C1-6 haloalkyl, or C1-6 haloalkoxy; Y represents halogeno, C1-6 alkyl, or C1-6 alkoxy; p is 0, 1/2, or 1; m and n each independently is an integer of 0 to 4; R1 represents C1-6 alkyl; R2 represents hydrogen, C1-6 alkyl, or C1-6 haloalkyl; and H-A represents an acid substance) are prepared and also disclosed are agricultural or horticultural fungicides containing the derivs. I as the active ingredient. Thus, 18.9 g K2CO3 and 13.9 g 2-chloromethyl-6-methylpyridine hydrochloride were added to a solution of 10.0 g N-[2-chloro-5-(1-hydroxyiminoethyl)benzyl]carbamic acid Me ester in 100 mL DMF and stirred at 90-100° for 8 h to give 8.2 g N-[2-chloro-5-[1-(6-methylpyridin-2-ylmethoxy)iminoethyl]benzyl]carbamic acid Me ester (II). II at 500 ppm completely controlled Erysiphe graminis in wheat seedlings.

IT 325155-92-8P, N-(2-Chloro-5-acetylbenzyl)carbamic acid methyl ester

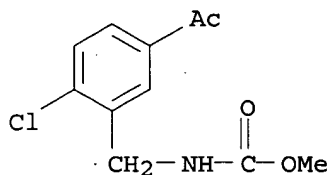
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of iminooxymethylpyridine compds. and agricultural or horticultural fungicides)

RN 325155-92-8 CAPLUS

CN Carbamic acid, [(5-acetyl-2-chlorophenyl)methyl]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:836782 CAPLUS

DOCUMENT NUMBER: 136:118413

TITLE: Anti-Helicobacter pylori Agents. 5. 2-(Substituted guanidino)-4-arylthiazoles and Aryloxazole Analogues

AUTHOR(S): Katsura, Yousuke; Nishino, Shigetaka; Inoue, Yoshikazu; Sakane, Kazuo; Matsumoto, Yoshimi; Morinaga, Chizu; Ishikawa, Hirohumi; Takasugi, Hisashi  
CORPORATE SOURCE: Medicinal Chemistry Research Laboratories and Medicinal Biology Research Laboratories, Fujisawa Pharmaceutical Company Ltd., Yodogawa-ku, Osaka, 532-8514, Japan

SOURCE: Journal of Medicinal Chemistry (2002), 45(1), 143-150  
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:118413

AB To extend the SAR study of guanidinothiazoles as a structurally novel class of anti-H. pylori agents, a series of 2-(substituted guanidino)-4-arylthiazoles and some 4-aryloxazole analogs were synthesized and evaluated for antimicrobial activity against H. pylori. Some of them were also subjected to H<sub>2</sub> antagonist and gastric antisecretory assays. Several arylthiazoles were identified as potent anti-H. pylori agents, and of these, a thienylthiazole derivative exhibited the strongest activity (MIC = 0.0065 µg/mL) among the compds. obtained in our guanidinothiazole studies. Although the thienylthiazole derivative was void of H<sub>2</sub> antagonist activity, a pyridylthiazole derivative had both potent anti-H. pylori and H<sub>2</sub> antagonist activities. On the other hand, no attractive activities were found in pyrimidyl, oxazolyl, isoxazolyl, imidazolyl, and oxadiazolylthiazole derivs. The anti-H. pylori activity of the aryloxazole analogs was weaker than those of the corresponding arylthiazole derivs., though they had potent H<sub>2</sub> antagonist activity.

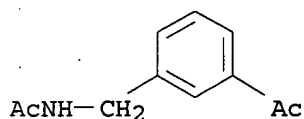
IT 149917-34-0 170634-23-8

RL: RCT (Reactant); RACT (Reactant or reagent)

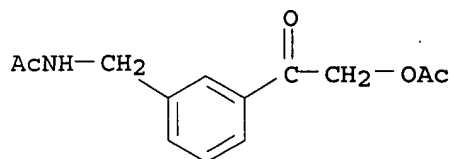
(preparation of guanidinoarylthiazoles and aryloxazoles and their antimicrobial activity against H. pylori., H<sub>2</sub> antagonist activity, and gastric antisecretory assays)

RN 149917-34-0 CAPLUS

CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



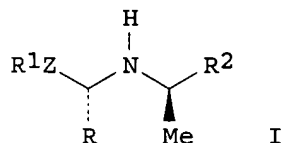
RN 170634-23-8 CAPLUS  
CN Acetamide, N-[[3-[(acetyloxy)acetyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2001:241760 CAPLUS  
DOCUMENT NUMBER: 134:280612  
TITLE: Preparation of 1-arylethylamines as calcium receptor ligands  
INVENTOR(S): Van Wagenen, Bradford C.; Moe, Scott T.; Balandrin, Manuel F.; Delmar, Eric G.; Nemeth, Edward F.  
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA  
SOURCE: U.S., 142 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6211244	B1	20010403	US 1995-546998	19951023
PRIORITY APPLN. INFO.:			US 1995-546998	19951023
OTHER SOURCE(S):	MARPAT 134:280612			

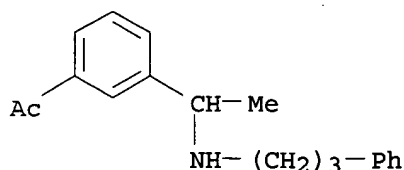


AB Title compds., e.g., I [R = H or alkyl; R1,R2 = (un)substituted Ph or naphthyl; Z = (CH2)0-3] were prepared Thus, (R)-1-(1-naphthyl)ethylamine was condensed with 2-acetonaphthone to give I (R = Me, R1 = 2-naphthyl, R2 = 1-naphthyl, Z = bond). Data for biol. activity of title compds. were given.

IT 159150-28-4P 332078-81-6P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of 1-arylethylamines as calcium receptor ligands)

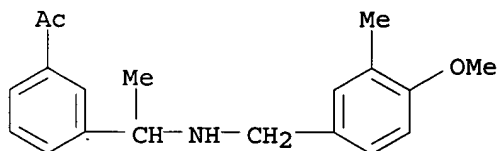
RN 159150-28-4 CAPLUS  
CN Ethanone, 1-[3-[1-[(3-phenylpropyl)amino]ethyl]phenyl]- (9CI) (CA INDEX

NAME)



RN 332078-81-6 CAPLUS

CN Ethanone, 1-[3-[1-[[4-methoxy-3-methylphenyl)methyl]amino]ethyl]phenyl]-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 229 THERE ARE 229 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:523449 CAPLUS

DOCUMENT NUMBER: 133:281719

TITLE: Anti-Helicobacter pylori Agents. 4. 2-(Substituted guanidino)-4-phenylthiazoles and Some Structurally Rigid Derivatives

AUTHOR(S): Katsura, Yousuke; Tomishi, Tetsuo; Inoue, Yoshikazu; Sakane, Kazuo; Matsumoto, Yoshimi; Morinaga, Chizu; Ishikawa, Hirohumi; Takasugi, Hisashi

CORPORATE SOURCE: Medicinal Chemistry Research Laboratories and Medicinal Biology Research Laboratories, Fujisawa Pharmaceutical Company Ltd., Osaka, 532-8514, Japan

SOURCE: Journal of Medicinal Chemistry (2000), 43(17), 3315-3321

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

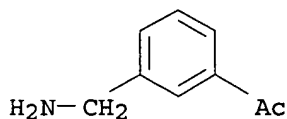
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:281719

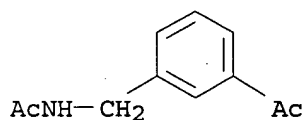
AB In order to find a new class of anti-Helicobacter pylori (H. pylori) agents, a series of 4-[(3-acetamido)phenyl]-2-(substituted guanidino)thiazoles and some structurally rigid analogs were synthesized and evaluated for antimicrobial activity against H. pylori. Among the compds. obtained, high anti-H. pylori activities were observed in N-[[3-[2-[[imino[(phenylmethyl)amino]methyl]amino]-4-thiazolyl]phenyl]methyl]acetamide (MIC = 0.025 µg/mL) and N-[[3-[2-[[imino[(2-phenylethyl)amino]methyl]amino]-4-thiazolyl]phenyl]methyl]acetamide (MIC = 0.037 µg/mL) and N-[[3-[2-[[imino[(2-(2-methoxyphenyl)ethyl)amino]methyl]amino]-4-thiazolyl]phenyl]methyl]acetamide (MIC = 0.017 µg/mL). Though alkyl derivs. generally showed lower activity, N-[[3-[2-[[imino[(2-methoxyethyl)amino]methyl]amino]-4-thiazolyl]phenyl]methyl]acetamide preserved significant activity (MIC = 0.32 µg/mL) and also exhibited more potent gastric antisecretory activity than ranitidine. Structural restriction by bridging between the thiazole and the Ph rings with an alkyl chain did not improve the activity in this series.

IT 149889-64-5P 149917-34-0P, N-[(3-Acetylphenyl)methyl]acetamide  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of (guanidino)phenylthiazoles and structurally rigid derivs.  
 for inhibition of Helicobacter pylori)  
 RN 149889-64-5 CAPLUS  
 CN Ethanone, 1-[3-(aminomethyl)phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

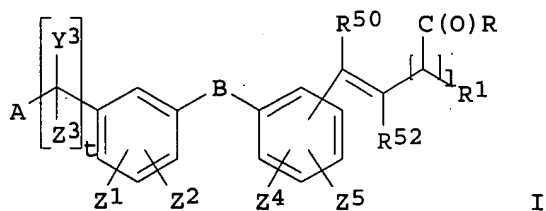
RN 149917-34-0 CAPLUS  
 CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



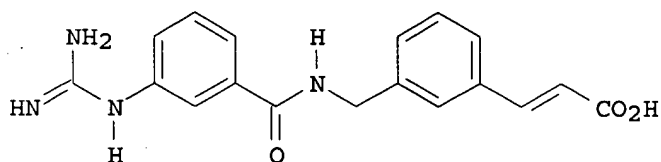
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1999:12345 CAPLUS  
 DOCUMENT NUMBER: 130:81288  
 TITLE: Preparation of cinnamic acid derivatives for selective  
 inhibiting or antagonizing the  $\alpha\text{v}\beta 3$   
 integrin  
 INVENTOR(S): Chen, Barbara B.; Chen, Helen Y.; Clare, Michael;  
 Docter, Stephen H.; Khanna, Ish Kumar; Koszyk, Francis  
 Jan; Malecha, James W.; Miyashiro, Julie Marion;  
 Penning, Thomas D.; Rico, Joseph G.; Ruminski, Peter  
 G.; Russell, Mark A.; Weier, Richard Mathias; Xu,  
 Xiangdong; Yu, Stella S.; Yu, Yi  
 PATENT ASSIGNEE(S): G.D. Searle and Co., USA  
 SOURCE: U.S., 77 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5852210	A	19981222	US 1997-825080	19970327
PRIORITY APPLN. INFO.:			US 1997-825080	19970327
OTHER SOURCE(S):	MARPAT 130:81288			
GI				



I



II

AB The title compds. [I; A = NR5C(:Y1)NR7R8 (wherein Y1 = NR2, O, S; R2 = H, alkyl, aryl, etc.; R7 = H, alkyl, alkenyl, etc.; R5 = H, alkyl, alkenyl, etc.; NR7R8 = (un)substituted 4-12 membered monocyclic or bicyclic ring containing 1 N atom), NR5C(Y2):NR7 (wherein Y2 = alkyl, cycloalkyl, bicycloalkyl, etc.), etc.; Z1, Z2, Z4, Z5 = H, alkyl, OH, etc.; B = CH:CH, CH2CONH, C(O)C:C, etc.; l = 0-3; t = 0-2; R50 = H, alkyl, aryl, etc.; R = XR3 (wherein X = O, S, NR4; R3, R4 = H, alkyl, alkenyl, etc.); Y3, Z3 = H, alkyl, aryl, etc.; R1 = H, alkyl, NH2, etc.; R52 = H, NHCO2R12, NSO2R12, etc.; R12 = H, alkyl, cycloalkyl, etc.] which selectively inhibit or antagonize the  $\alpha\beta 3$  integrin, and are useful in treating tumor metastasis, solid tumor growth, angiogenesis, osteoporosis, humoral hypercalcemia of malignancy, smooth muscle cell migration, and restenosis, were prepared Thus, a 5-step synthesis of II, starting with 3-bromobenzylamine.HCl, which showed IC50 of 13.0 nM against  $\alpha\beta 3$  vs. IC50 of 657 nM against IIB/IIIa.

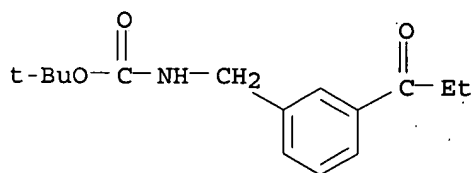
IT 198195-10-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cinnamic acid derivs. for selective inhibiting or antagonizing the  $\alpha\beta 3$  integrin)

RN 198195-10-7 CAPLUS

CN Carbamic acid, [[3-(1-oxopropyl)phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:338370 CAPLUS

DOCUMENT NUMBER: 129:27906

TITLE: Inhibitors of Acyl-CoA:Cholesterol O-Acyltransferase. Part 2. Identification and Structure-Activity Relationships of a Novel Series of N-Alkyl-N-(heteroaryl-substituted benzyl)-N'-arylureas

AUTHOR(S): Tanaka, Akira; Terasawa, Takeshi; Hagihara, Hiroyuki; Sakuma, Yuri; Ishibe, Noriko; Sawada, Masae; Takasugi, Hisashi; Tanaka, Hirokazu

CORPORATE SOURCE: Medicinal Chemistry Research Laboratories, Fujisawa Pharmaceutical Co. Ltd., Osaka, 532, Japan

SOURCE: Journal of Medicinal Chemistry (1998), 41(13), 2390-2410  
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

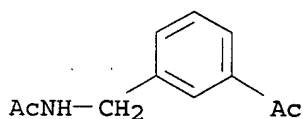
LANGUAGE: English

AB A series of N-alkyl-N-(heteroaryl-substituted benzyl)-N'-arylurea and related derivs. have been prepared and evaluated for their ability to inhibit acyl-CoA:cholesterol O-acyltransferase in vitro and to lower plasma cholesterol levels in cholesterol-fed rats in vivo. A pyrazol-3-yl group on the N-benzyl group was identified as a heteroarom. ring providing a good profile of biol. activity. As a result of optimization of the combination with the N-alkyl group and N-aryl group, compound FR186054 was identified as a new, orally efficacious ACAT inhibitor, which exhibited potent in vitro ACAT inhibitory activity (rabbit intestinal microsomes IC50 = 99 nM) and excellent hypocholesterolemic effects in cholesterol-fed rats, irresp. of administration mode (ED50 = 0.046 mg/kg dosed via the diet, ED50 = 0.44 mg/kg administered by gavage in PEG400 vehicle). Moreover, a toxicol. study revealed this compound to be nontoxic to the adrenal glands of dogs when tested at a single dose of 10 mg/kg po.

IT 149917-34-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of alkyl(heteroaryl-substituted benzyl)arylureas as acyl-CoA:cholesterol O-acyltransferase inhibitors)

RN 149917-34-0 CAPLUS

CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:455768 CAPLUS

DOCUMENT NUMBER: 125:114322

TITLE: Preparation of urea derivatives as cholesterol acyltransferase inhibitors

INVENTOR(S): Terasawa, Takeshi; Tanaka, Akira; Chiba, Toshiyuki; Takasugi, Hisashi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 228 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9610559	A1	19960411	WO 1995-JP1982	19950929
W: AU, CA, CN, HU, JP, KR, MX, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2200981	AA	19960411	CA 1995-2200981	19950929

AU 9535779	A1	19960426	AU 1995-35779	19950929
EP 784612	A1	19970723	EP 1995-932934	19950929
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 10510512	T2	19981013	JP 1995-511616	19950929
ZA 9508365	A	19960508	ZA 1995-8365	19951004
PRIORITY APPLN. INFO.:			GB 1994-19970	A 19941004
			GB 1995-6720	A 19950331
			GB 1995-14021	A 19950710
			WO 1995-JP1982	W 19950929

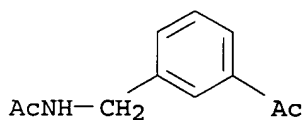
OTHER SOURCE(S): MARPAT 125:114322

AB R4YC6H4(CH2)nNR2CONHR3 [R2 = (ar)alkyl, heterocyclyl(alkyl), alkoxyalkyl, etc.; R3,R4 = (un)substituted aryl, heterocyclyl; Y = bond, alkylene, O, CO, CONH, etc.; n = 0 or 1] were prepare Thus, 1-cycloheptyl-1-(4-phenoxyphenylmethyl)-3-(2,4,6-trifluorophenyl)urea had IC50 of 1.1x10-8M against cholesterol acyltransferase in vitro.

IT 149917-34-0, N-(3-Acetylbenzyl)acetamide  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of urea derivs. as cholesterol acyltransferase inhibitors)

RN 149917-34-0 CAPLUS

CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



L15 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:392101 CAPLUS

DOCUMENT NUMBER: 125:96084

TITLE: Aromatic compounds containing basic and acidic termini useful as fibrinogen receptor antagonists

INVENTOR(S): Cain, Gary A.; Eyermann, Charles J.

PATENT ASSIGNEE(S): Du Pont Merck Pharmaceutical Co., USA

SOURCE: U.S., 43 pp.  
 CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5523302	A	19960604	US 1993-157860	19931124
US 5739163	A	19980414	US 1996-612597	19960308
PRIORITY APPLN. INFO.:			US 1993-157860	A3 19931124

OTHER SOURCE(S): MARPAT 125:96084

AB This invention relates to novel compds. containing basic and acidic termini, pharmaceutical compns. containing such compds., processes for preparing such compds., and methods of using these compds., alone or in combination with other therapeutic agents, for the inhibition of platelet aggregation, as thrombolytics, and/or for the treatment of thromboembolic disorders.

IT 179002-56-3P 179002-58-5P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (aromatic compds. containing basic and acidic termini useful as fibrinogen receptor antagonists)

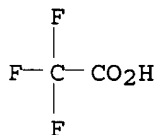
RN 179002-56-3 CAPLUS

CN Acetic acid, 2,2'-[[4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-1,2-phenylene]bis(oxy)]bis-, (E)-, trifluoroacetate (9CI) (CA INDEX NAME)

CRN 179000-32-9  
CMF C20 H19 N 07

NCC1=CC=C(C(=O)C/C=C/C2=CC=C(OC(=O)C)OC(=O)C)C=C1

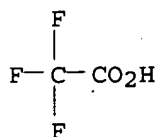
CRN 76-05-1  
CMF C2 H F3 O2



CRN 179000-68-1  
CMF C20 H21 N3 O5

NC(=N)NCc1ccc(cc1)C(=O)/C=C/c2ccc(OC)c(OCOC(=O)O)c2

CRN 76-05-1  
CMF C2 H F3 O2



IT 179000-32-9 179000-33-0 179000-34-1  
 179000-35-2 179000-36-3 179000-37-4  
 179000-41-0 179000-42-1 179000-43-2  
 179000-44-3 179000-68-1 179000-69-2  
 179000-70-5 179000-91-0 179002-51-8

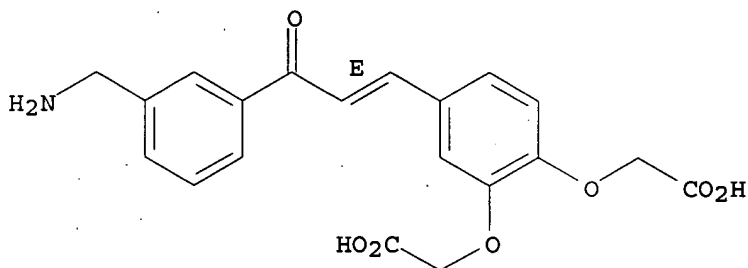
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(aromatic compds. containing basic and acidic termini useful as fibrinogen receptor antagonists)

RN 179000-32-9 CAPLUS

CN Acetic acid, 2,2'-[[4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-1,2-phenylene]bis(oxy)]bis-, (E)- (9CI) (CA INDEX NAME)

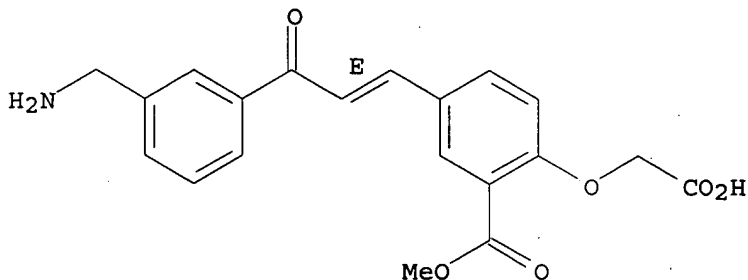
Double bond geometry as shown.



RN 179000-33-0 CAPLUS

CN Benzoic acid, 5-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-2-(carboxymethoxy)-, 1-methyl ester, (E)- (9CI) (CA INDEX NAME)

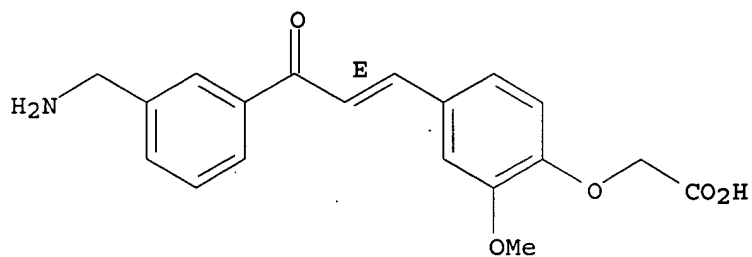
Double bond geometry as shown.



RN 179000-34-1 CAPLUS

CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-2-methoxyphenoxy]-, (E)- (9CI) (CA INDEX NAME)

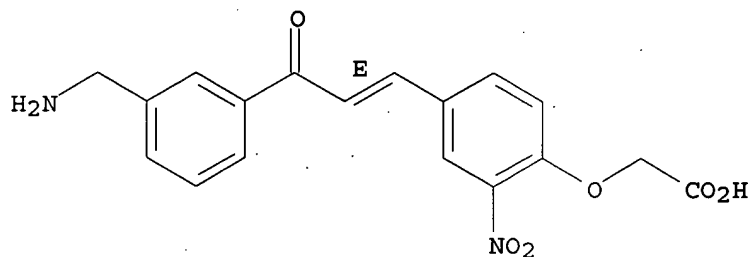
Double bond geometry as shown.



RN 179000-35-2 CAPLUS

CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-2-nitrophenoxy]-, (E)- (9CI) (CA INDEX NAME)

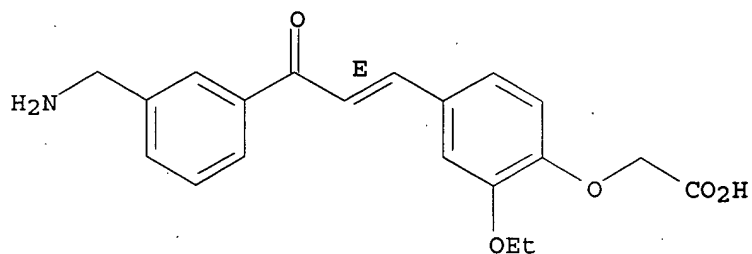
Double bond geometry as shown.



RN 179000-36-3 CAPLUS

CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-2-ethoxyphenoxy]-, (E)- (9CI) (CA INDEX NAME)

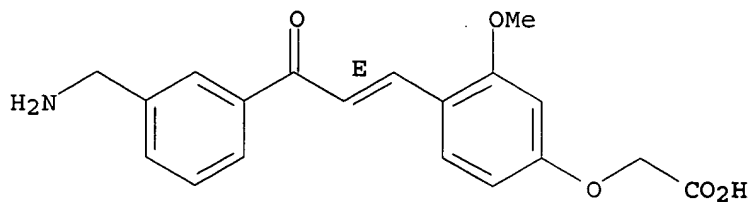
Double bond geometry as shown.



RN 179000-37-4 CAPLUS

CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-3-methoxyphenoxy]-, (E)- (9CI) (CA INDEX NAME)

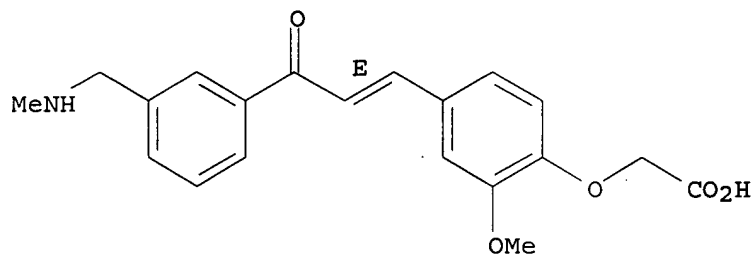
Double bond geometry as shown.



RN 179000-41-0 CAPLUS

CN Acetic acid, [2-methoxy-4-[3-[3-[(methylamino)methyl]phenyl]-3-oxo-1-propenyl]phenoxy]-, (E)- (9CI) (CA INDEX NAME)

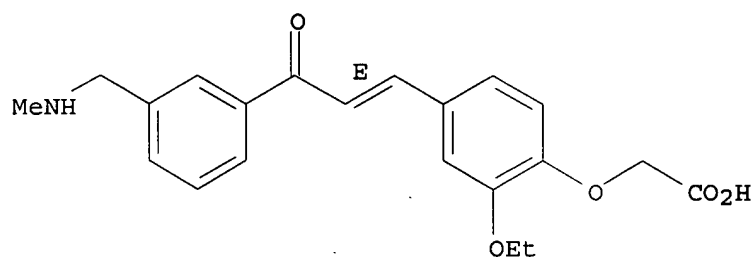
Double bond geometry as shown.



RN 179000-42-1 CAPLUS

CN Acetic acid, [2-ethoxy-4-[3-[3-[(methylamino)methyl]phenyl]-3-oxo-1-propenyl]phenoxy]-, (E)- (9CI) (CA INDEX NAME)

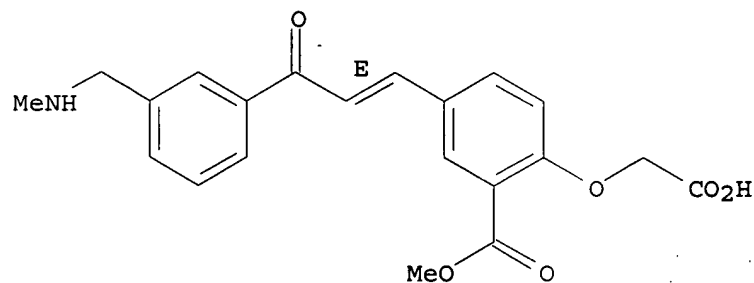
Double bond geometry as shown.



RN 179000-43-2 CAPLUS

CN Benzoic acid, 2-(carboxymethoxy)-5-[3-[3-[(methylamino)methyl]phenyl]-3-oxo-1-propenyl]-, 1-methyl ester, (E)- (9CI) (CA INDEX NAME)

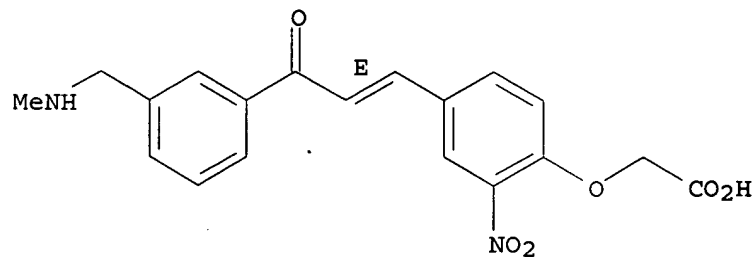
Double bond geometry as shown.



RN 179000-44-3 CAPLUS

CN Acetic acid, [4-[3-[3-[(methylamino)methyl]phenyl]-3-oxo-1-propenyl]-2-nitrophenoxy]-, (E)- (9CI) (CA INDEX NAME)

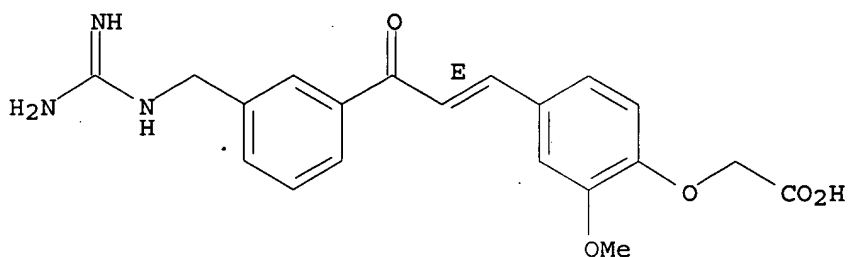
Double bond geometry as shown.



RN 179000-68-1 CAPLUS

CN Acetic acid, [4-[3-[3-[[[(aminoiminomethyl)amino]methyl]phenyl]-3-oxo-1-propenyl]-2-methoxyphenoxy]-, (E)- (9CI) (CA INDEX NAME)

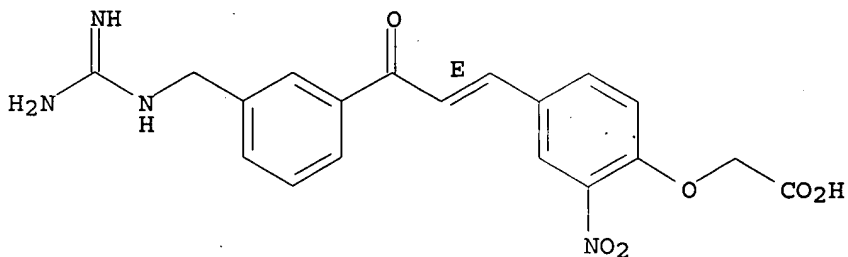
Double bond geometry as shown.



RN 179000-69-2 CAPLUS

CN Acetic acid, [4-[3-[3-[[[(aminoiminomethyl)amino]methyl]phenyl]-3-oxo-1-propenyl]-2-nitrophenoxy]-, (E)- (9CI) (CA INDEX NAME)

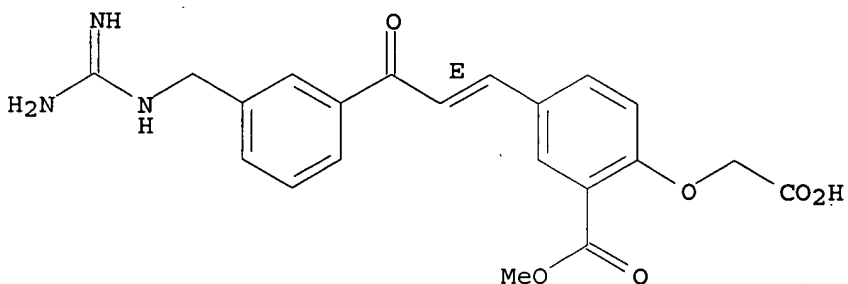
Double bond geometry as shown.



RN 179000-70-5 CAPLUS

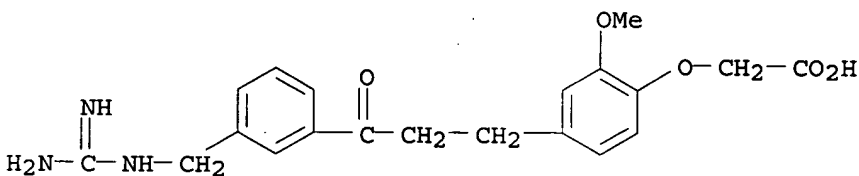
CN Benzoic acid, 5-[3-[3-[[[(aminoiminomethyl)amino]methyl]phenyl]-3-oxo-1-propenyl]-2-(carboxymethoxy)-, 1-methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



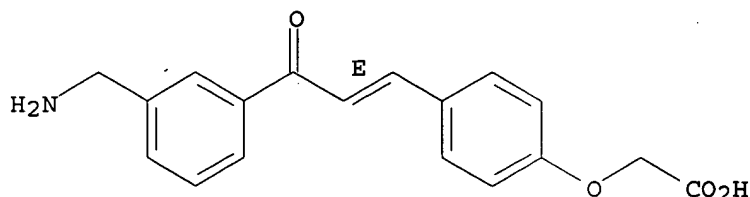
RN 179000-91-0 CAPLUS

CN Acetic acid, [4-[3-[3-[[[(aminoiminomethyl)amino]methyl]phenyl]-3-oxopropyl]-2-methoxyphenoxy]- (9CI) (CA INDEX NAME)



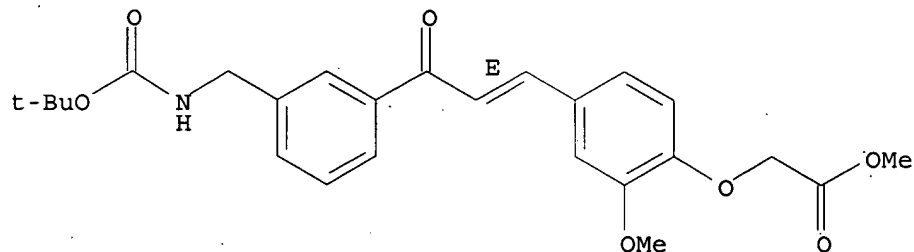
RN 179002-51-8 CAPLUS  
 CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]phenoxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT 179003-03-3P 179003-05-5P 179003-06-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (aromatic compds. containing basic and acidic termini useful as fibrinogen receptor antagonists)  
 RN 179003-03-3 CAPLUS  
 CN Acetic acid, [4-[3-[3-[[[(1,1-dimethylethoxy)carbonyl]amino]methyl]phenyl]-3-oxo-1-propenyl]-2-methoxyphenoxy]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

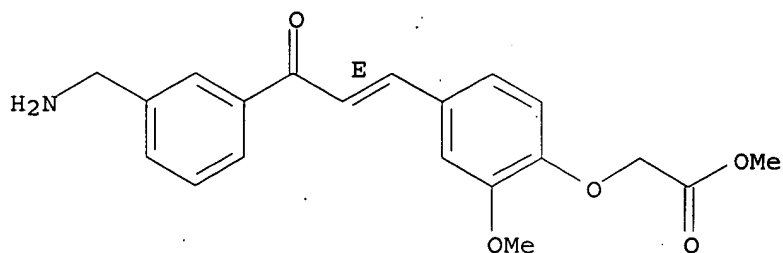


RN 179003-05-5 CAPLUS  
 CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-2-methoxyphenoxy]-, methyl ester, (E)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

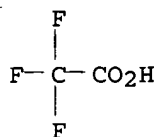
CRN 179003-04-4  
 CMF C20 H21 N O5

Double bond geometry as shown.



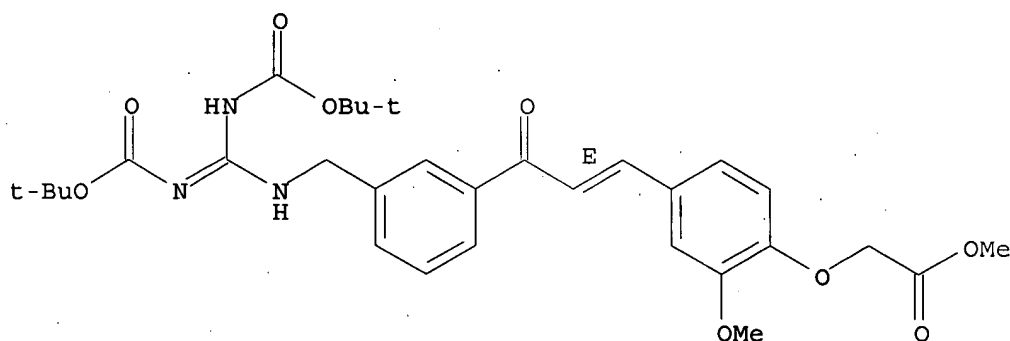
CM 2

CRN 76-05-1  
CMF C2 H F3 O2



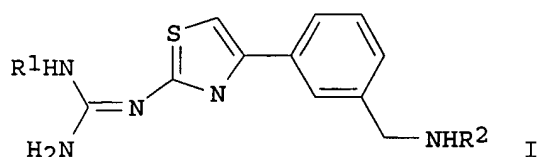
RN 179003-06-6 CAPLUS  
CN Acetic acid, [4-[3-[3-[[[bis[[[(1,1-dimethylethoxy)carbonyl]amino]methylene]amino]methyl]phenyl]-3-oxo-1-propenyl]-2-methoxyphenoxy]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as described by E or Z.



L15 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1996:385930 CAPLUS  
DOCUMENT NUMBER: 125:58498  
TITLE: Preparation of 4-(3-aminomethylphenyl)-2-thiazolylguanidines as H2-receptor antagonists  
INVENTOR(S): Katsura, Yousuke; Tomishi, Tetsuo; Nishino, Shigetaka; Ohno, Mitsuko  
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan  
SOURCE: PCT Int. Appl., 34 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9605187	A1	19960222	WO 1995-JP1596	19950809
W: AU, BR, CA, CN, FI, HU, JP, KR, MX, NO, NZ, RU, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9531929	A1	19960307	AU 1995-31929	19950809
JP 2000504305	T2	20000411	JP 1995-507193	19950809
PRIORITY APPLN. INFO.:			GB 1994-16459	A 19940815
			WO 1995-JP1596	W 19950809
OTHER SOURCE(S):	MARPAT	125:58498		
GI				

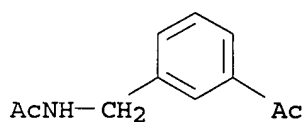


AB Title compds. [I; R1 = alkoxy(alkyl), cyanoalkyl, phenyl(oxy)(alkyl), etc.; R2 = H, alkanoyl, CONH2] were prepared Thus, I [R1 = 2-(1-cyclohexenyl)ethyl, R2 = Ac] gave 100% inhibition of histamine-induced increase of guinea pig atrial strip contraction at 10-6g/mL in vitro.

IT 149917-34-0, 3-(Acetylaminomethyl)acetophenone  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of 4-(3-aminomethylphenyl)-2-thiazolylguanidines as H2-receptor antagonists)

RN 149917-34-0 CAPLUS

CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



L15 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:934019 CAPLUS

DOCUMENT NUMBER: 123:340105

TITLE: Preparation of oxazole derivatives as bactericides and ulcer inhibitors

INVENTOR(S): Katsura, Yosuke; Inoe, Zenichi; Fuji, Tetsuo; Takasugi, Hisashi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.  
 CODEN: JKXXAF

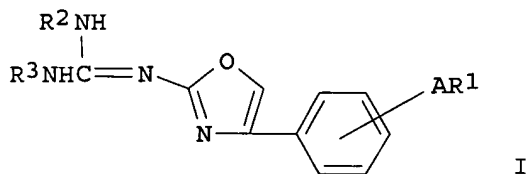
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 07188197	A2	19950725	JP 1994-303222	19941110
PRIORITY APPLN. INFO.:			JP 1994-303222	A 19941110
			JP 1993-312542	19931117
OTHER SOURCE(S):	MARPAT 123:340105			
GI				



AB The title compds. I [R1 = (un)substituted amino; R2, R3 = H, (un)substituted aliphatic hydrocarbon, etc.; A = alkylene] are prepared

4-(3-Acetylaminomethylphenyl)-2-[(amino)(2-methoxybenzylamino)methyleneamino]oxazole (preparation given) in vitro showed MIC of 0.182 µg/mL against *Helicobacter Pylori*. The MICs of 3 three other compds. of this invention against *Helicobacter Pylori* are also given this document.

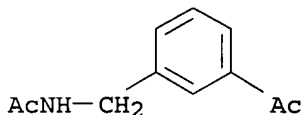
IT 149917-34-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of oxazole derivs. as bactericides and ulcer inhibitors)

RN 149917-34-0 CAPLUS

CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



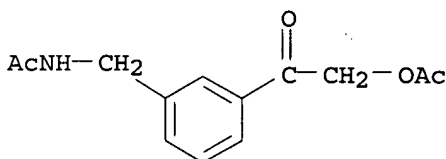
IT 170634-23-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of oxazole derivs. as bactericides and ulcer inhibitors)

RN 170634-23-8 CAPLUS

CN Acetamide, N-[[3-[(acetyloxy)acetyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



L15 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:436152 CAPLUS

DOCUMENT NUMBER: 121:36152

TITLE: Template-Constrained Cyclic Peptides: Design of High-Affinity Ligands for GPIIb/IIIa

AUTHOR(S): Jackson, Sharon; DeGrado, W.; Dwivedi, A.; Parthasarathy, A.; Higley, A.; Krywko, J.; Rockwell, A.; Markwalder, J.; Wells, G.; et al.

CORPORATE SOURCE: Experimental Station, DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0328, USA

SOURCE: Journal of the American Chemical Society (1994), 116(8), 3220-30

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

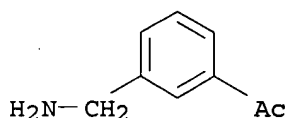
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The general strategy of tying amino and carboxy terminal ends of a peptide onto a semirigid template to lock the intervening peptide backbone into a single conformer or a family of related conformers was tested using the tripeptide sequence Arg-Gly-Asp (RGD), which binds with low affinity to the platelet glycoprotein IIb/IIIa (GPIIb/IIIa). Mimics of RGD are of interest as antithrombotics because of their ability to inhibit the aggregation of platelets. Prior to this study, J. Samanen; et al. (1991) prepared disulfide-containing cyclic pentapeptide I (MeArg = N-methyl-L-arginine, Pen = L-penicillamine) (SK&F 106760) that bound to GPIIb/IIIa with an affinity of approx. 0.1 µM. NMR anal. of the solution conformation of I suggested that replacing the disulfide-containing portion of the cycle with m-(aminomethyl)benzoic acid would lead to a more rigid structure. 39Indeed, introduction of this template into a cyclic RGD-containing peptide resulted in compds. with high affinity for the

receptor. Further, systematic inclusion of addnl. conformational constraints in the form of N $\alpha$ - and C $\alpha$ -alkyl groups led to peptide II with an affinity of approx. 100 pM for binding to the receptor. II also showed good activity in the platelet aggregation assay at oral doses as low as 0.1 mg/kg.

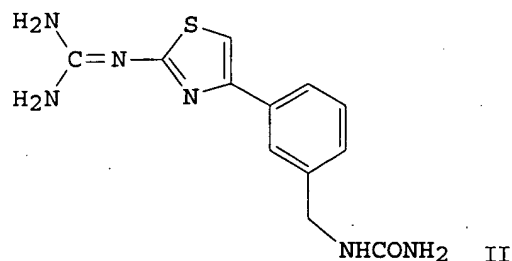
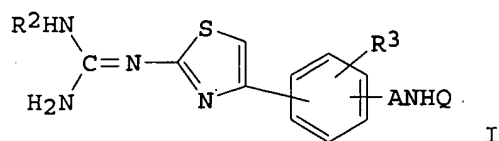
IT 149889-64-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and butoxycarbonylation of)  
 RN 149889-64-5 CAPLUS  
 CN Ethanone, 1-[3-(aminomethyl)phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L15. ANSWER 13 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1993:603405 CAPLUS  
 DOCUMENT NUMBER: 119:203405  
 TITLE: Preparation of guanidinothiazoles and their use as histamine H<sub>2</sub>-receptor antagonists  
 INVENTOR(S): Katsura, Yousuke; Tomishi, Tetsuo; Inoue, Yoshikazu; Takasugi, Hisashi  
 PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan  
 SOURCE: Eur. Pat. Appl., 49 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 545376	A1	19930609	EP 1992-120533	19921202
EP 545376	B1	19980909		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
ZA 9208876	A	19930715	ZA 1992-8876	19921117
AU 9229837	A1	19930610	AU 1992-29837	19921202
AU 666893	B2	19960229		
JP 06321921	A2	19941122	JP 1992-323052	19921202
JP 2531329	B2	19960904		
AT 170851	E	19980915	AT 1992-120533	19921202
CA 2084640	AA	19930607	CA 1992-2084640	19921204
HU 65776	A2	19940728	HU 1992-3849	19921204
CN 1079469	A	19931215	CN 1992-114939	19921205
US 5532258	A	19960702	US 1994-356967	19941216
PRIORITY APPLN. INFO.:			GB 1991-25970	A 19911206
			US 1992-978477	B1 19921118
OTHER SOURCE(S):	MARPAT 119:203405			
GI				



AB Title compds. [I; R2 = H, (substituted) alkyl; R3 = H, alkyl, alkoxy, halo; A = alkylene; Q = COR1, (substituted) carbamimidoyl; R1 = organic group], were prepared. Thus, 4-(3-aminomethylphenyl)-2-(diaminomethyleneamino)thiazole dihydrochloride (preparation given) was stirred with potassium isocyanate in H2O at room temperature for 8.5 h to give title compound II. II at 1 mg/kg i.v. in rats inhibited 99% gastric acid secretion.

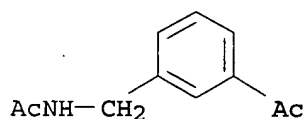
IT 149917-34-0P 149917-44-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for guanidinothiazole derivative hiatamine receptor H2 antagonist)

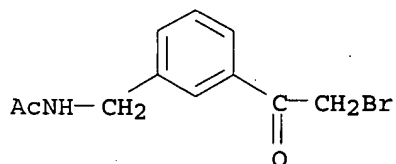
RN 149917-34-0 CAPLUS

CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 149917-44-2 CAPLUS

CN Acetamide, N-[[3-(bromoacetyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



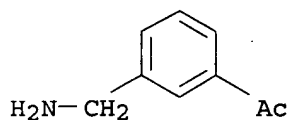
IT 149889-64-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of guanidinothiazole H2 antagonist)

RN 149889-64-5 CAPLUS

CN Ethanone, 1-[3-(aminomethyl)phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L15 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:449076 CAPLUS

DOCUMENT NUMBER: 119:49076

TITLE: Preparation of phenylacetamide derivatives as acyl Co-A-cholesterol acyltransferase (ACAT) inhibitors

INVENTOR(S): Sano, Mitsuharu; Chihara, Yasuaki; Ikezawa, Ryuhei; Ooe, Takanori; Kusuhara, Hidenobu; Izumi, Noritaka

PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

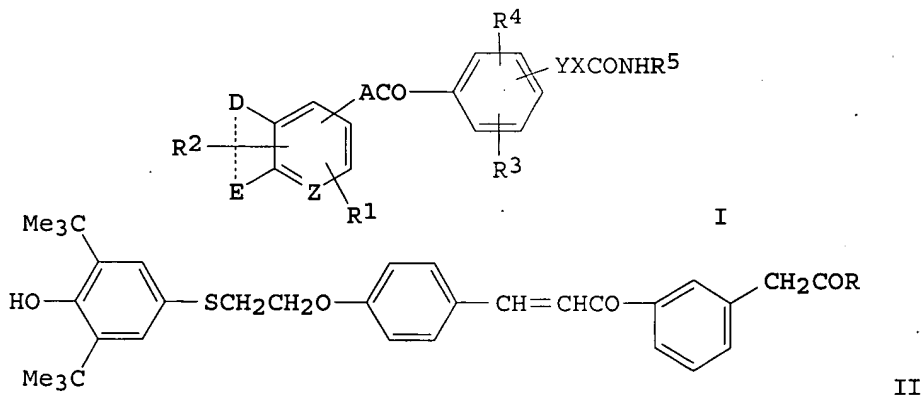
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05025115	A2	19930202	JP 1991-203857	19910717
PRIORITY APPLN. INFO.:			JP 1991-203857	19910717
OTHER SOURCE(S):	CASREACT 119:49076; MARPAT 119:49076			

GI



AB The title compds. [I; R1, R2 = H, halo, alkyl, alkoxy, aryloxy, aralkoxy, etc.; R3, R4 = H, halo, alkyl, alkoxy; R5 = (substituted) aryl; A = alkylene, alkenylene; Z = CH, N; Y = alkylene, oxyalkylene; X = bond, NH; DE may form a ring], useful as anticholesteremics and arteriosclerotics, are prepared Et3N was added to a solution of acid II (R = OH) in EtOAc, followed by pivaloyl chloride with stirring at 0-5°, 2,6-Et2C6H3NH2 was added at 0-5°, and the mixture was stirred at room temperature to give amide II (R = 2,6-Et2C6H3NH). Also prepared were 27 addnl. I, which showed IC50 of 0.02-0.07  $\mu$ M against ACAT and lowered liver cholesterol by 35-61% in rats at 0.01-0.1% in feed.

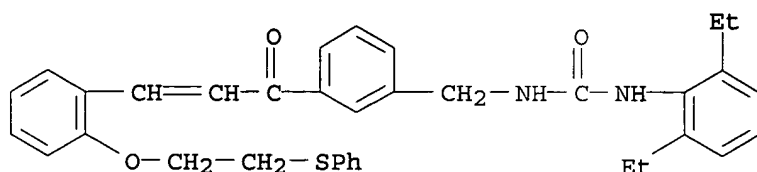
IT 148491-56-9P 148491-58-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as anticholesteremic and arteriosclerotic agent)

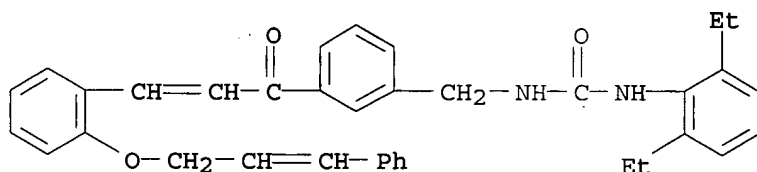
RN 148491-56-9 CAPLUS

CN Urea, N-(2,6-diethylphenyl)-N'-[[3-[1-oxo-3-[2-[2-(phenylthio)ethoxy]phenyl]-2-propenyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 148491-58-1 CAPLUS

CN Urea, N-(2,6-diethylphenyl)-N'-[[3-[1-oxo-3-[2-[(3-phenyl-2-propenyl)oxy]phenyl]-2-propenyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



=> s l3 and aluminum

757 L3

955395 ALUMINUM

L16

3 L3 AND ALUMINUM

=> d l16 ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):1

YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y

L16 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:722822 CAPLUS

DOCUMENT NUMBER: 141:239312

TITLE: Compositions and methods for detection and isolation of phosphorylated molecules

INVENTOR(S): Agnew, Brian; Beechem, Joseph; Gee, Kyle; Haugland, Richard; Steinberg, Thomas; Patton, Wayne

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 89 pp., Cont.-in-part of U.S. Ser. No. 428,192.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004171034	A1	20040902	US 2003-703816	20031107
US 2004038306	A1	20040226	US 2003-428192	20030502
US 7102005	B2	20060905		
CA 2483868	AA	20040521	CA 2003-2483868	20030502
AU 2003299466	A1	20040607	AU 2003-299466	20030502
EP 1546118	A2	20050629	EP 2003-799756	20030502

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 JP 2005539243 T2 20051222 JP 2004-549877 20030502  
 US 2005014197 A1 20050120 US 2004-821522 20040409  
 WO 2005047901 A2 20050526 WO 2004-US36968 20041105  
 WO 2005047901 A3 20050728

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,  
 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,  
 GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,  
 LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,  
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,  
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, AM,  
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,  
 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO,  
 SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,  
 NE, SN, TD, TG

PRIORITY APPLN. INFO.:

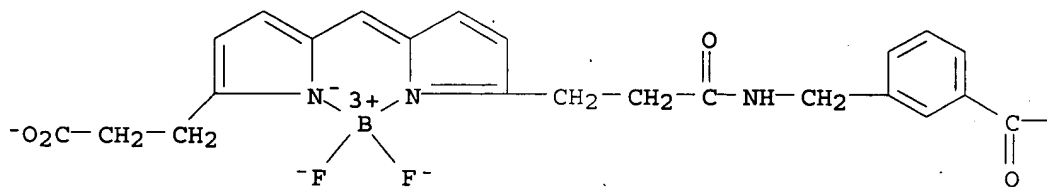
US 2002-377733P P 20020503  
 US 2002-393059P P 20020628  
 US 2002-407255P P 20020830  
 US 2003-440252P P 20030114  
 US 2003-428192 A2 20030502  
 WO 2003-US13765 W 20030502  
 US 2003-703816 A2 20031107

AB The present invention relates to phosphate-binding compds. that find use in binding, detecting and isolating phosphorylated target mols. including the subsequent identification of target mols. that interact with phosphorylated target mols. or mols. capable of being phosphorylated. A binding solution is provide that comprises a phosphate-binding compound, an acid and a metal ion wherein the metal ion simultaneously interacts with an exposed phosphate group on a target mol. and the metal chelating moiety of the phosphate-binding compound forming a bridge between the phosphate-binding compound and a phosphorylated target mol. resulting in a ternary complex. The binding solution of the present invention finds use in binding and detecting immobilized and solubilized phosphorylated target mols., isolation of phosphorylated target mols. from a complex mixture and aiding in proteomic anal. wherein kinase and phosphatase substrates and enzymes can be identified.

IT 749863-24-9P 749863-26-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (compns. and methods for detection and isolation of phosphorylated mols.)

RN 749863-24-9 CAPLUS  
 CN Borate(1-), [5-[[[5-[3-[[[3-benzoylphenyl)methyl]amino]-3-oxopropyl]-2H-pyrrol-2-ylidene-κN]methyl]-1H-pyrrole-2-propanoato(2-)-κN1]difluoro-, hydrogen, (T-4)-(9CI) (CA INDEX NAME)

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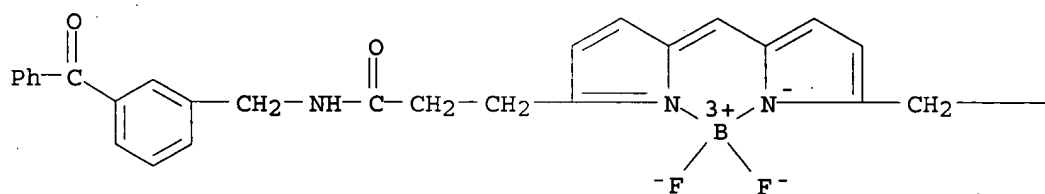
● H<sup>+</sup>

— Ph

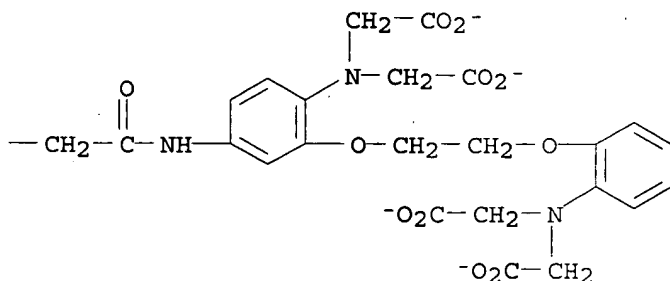
RN 749863-26-1 CAPLUS

CN Borate(4-), [N-[2-[2-[5-[[3-[5-[[5-[3-[[[3-benzoylphenyl)methyl]amino]-3-oxopropyl]-2H-pyrrol-2-ylidene-κN)methyl]-1H-pyrrol-2-yl-κN]-1-oxopropyl]amino]-2-[bis(carboxymethyl)amino]phenoxy]ethoxy]phenyl]-N-(carboxymethyl)glycinato(5-)]difluoro-, tetrasodium, (T-4)-(9CI) (CA INDEX NAME)

PAGE 1-A

● 4 Na<sup>+</sup>

PAGE 1-B



L16 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:610021 CAPLUS

DOCUMENT NUMBER: 141:153045

TITLE: Fluorescent assays for screening for protein kinase inhibitors applicable in cancer treatment and diagnosis

INVENTOR(S): Lawrence, David S.

PATENT ASSIGNEE(S): Albert Einstein College of Medicine of Yeshiva University, USA

SOURCE: PCT Int. Appl., 188 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004062475	A2	20040729	WO 2004-US480	20040109
WO 2004062475	A3	20050901		
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ				
US 2005054024	A1	20050310	US 2004-755086	20040109
PRIORITY APPLN. INFO.:			US 2003-439359P	P 20030110
			US 2003-505097P	P 20030922

OTHER SOURCE(S): MARPAT 141:153045

AB This invention provides fluorescently-labeled peptide substrates for protein kinases; methods using the substrates for identifying compds. that inhibit protein kinases, for determining if particular protein kinases are active in cells, for diagnosing diseases, and for preparing compns.; and compns. comprising the substrates. Several schemes for the synthesis of protein kinase C fluorescently-labeled peptide substrates, adaptable to the preparation of large peptide libraries, are provided. In particular embodiments, a library of fluorescently labeled protein kinase C (PKC) peptide substrates was prepared to identify a phosphorylation-induced reporter of protein kinase activity. The lead PKC substrate displays a 2.5-fold change in fluorescence intensity upon phosphorylation. PKC activity can also be detected in cell lysates containing the activated PKCs and living cells. Immunodepletion of conventional PKCs from the cell lysate eliminates the fluorescence response, suggesting that this peptide substrate is selectively phosphorylated by PKC $\alpha$ ,  $\beta$ , and  $\gamma$ . Finally, living cells microinjected with the peptide substrate exhibit a 2-fold increase in fluorescence intensity upon exposure to a PKC activator. Thus this peptide based protein kinase biosensors is useful in monitoring the temporal and spatial dynamics of PKC activity in living cells, and applicable in cancer treatment and diagnosis.

IT 728044-64-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

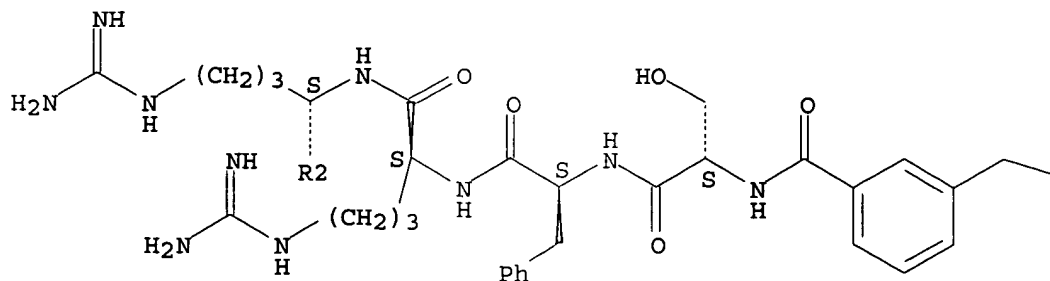
(fluorescent assays for screening for protein kinase inhibitors applicable in cancer treatment and diagnosis)

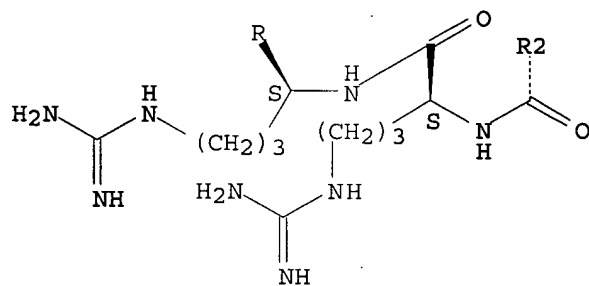
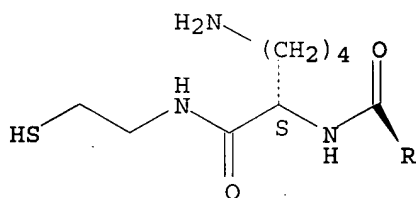
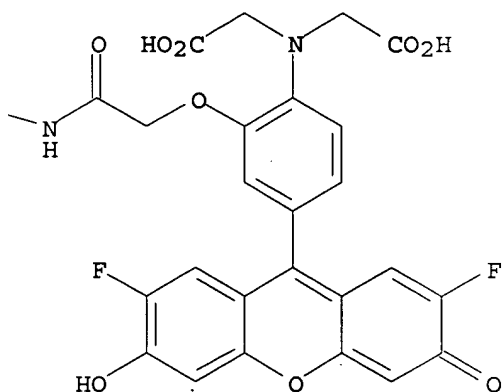
RN 728044-64-2 CAPLUS

CN L-Lysinamide, N-[3-[[[2-[bis(carboxymethyl)amino]-5-(2,7-difluoro-6-hydroxy-3-oxo-3H-xanthen-9-yl)phenoxy]acetyl]amino]methyl]benzoyl]-L-seryl-L-phenylalanyl-L-arginyl-L-arginyl-L-arginyl-L-arginyl-N-(2-mercaptoethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





IT 2393-20-6  
 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES  
 (Uses)  
 (linker in PKC peptide substrate; fluorescent assays for screening for  
 protein kinase inhibitors applicable in cancer treatment and diagnosis)  
 RN 2393-20-6 CAPLUS  
 CN Benzoic acid, 3-(aminomethyl)- (9CI) (CA INDEX NAME)

